2-Methylheptane
592-27-8 | DTXSID2060460

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.96

Global applicability domain: Inside

Local applicability domain index: 9.74e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

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Hexanenitrile
Measured: 4.08
Predicted: 3.96

Image not found

Dimethyl sulfoxide
Measured: 4.96
Predicted: 3.99

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3-Methylbutyl acetate
Measured: 3.94
Predicted: 3.63

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Toluene
Measured: 3.31
Predicted: 3.87

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1-Octene
Measured: 3.35
Predicted: 3.48